

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

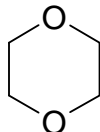
1,4-Dioxane or para-dioxane is also commonly referred as simply 'dioxane'. However, 1,4-dioxane should not be confused with dioxin (or dioxins), which are a different class of chemical compounds. Information regarding the chemical identity of 1,4-dioxane is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

1,4-Dioxane is a colorless volatile liquid. 1,4-Dioxane is also completely miscible in water and organic solvents. The technical-grade product is >99.9% pure, but may contain bis(2-chloroethyl) ether as an impurity (DeRosa et al. 1996). Information regarding the physical and chemical properties of 1,4-dioxane is located in Table 4-2.

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Table 4-1. Chemical Identity of 1,4-Dioxane

| Characteristic | Information |
|--------------------------|--|
| Chemical name | 1,4-Dioxane |
| Synonym(s) | 1,4-diethylenedioxide; 1,4-dioxacyclohexane; 1,4-dioxanne (French); di(ethylene oxide); diethylene dioxide; diethylene ether; dioksan (Polish); diossano-1,4 (Italian); dioxaan-1,4 (Dutch); dioxan; dioxan-1,4 (German); dioxane; dioxane-1,4; dioxanne (French); dioxyethylene ether; glycol ethylene ether; para-dioxane; <i>p</i> -dioxan (Czech); <i>p</i> -dioxane; <i>p</i> -dioxin, tetrahydro-; tetrahydro-1,4-dioxin; tetrahydro-para-dioxin; tetrahydro- <i>p</i> -dioxin |
| Registered trade name(s) | No data |
| Chemical formula | C ₄ H ₈ O ₂ |
| Chemical structure |  |
| Identification numbers: | |
| CAS Registry | 123-91-1 |
| NIOSH RTECS | JG8225000 |
| EPA Hazardous Waste | U108; A toxic waste when a discarded commercial chemical product or manufacturing chemical intermediate or an off-specification commercial chemical product or a manufacturing chemical intermediate |
| OHM/TADS | No data |
| DOT/UN/NA/IMCO | UN 1165; IMO 3.2 |
| HSDB | 81 |
| NCI | No data |

CAS = Chemical Abstracts Services; CIS = Chemical Information System; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substance Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

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Table 4-2. Physical and Chemical Properties of 1,4-Dioxane

| Property | |
|--------------------------------------|--|
| Molecular weight (g/mol) | 88.11 ^a |
| Color | Clear ^b |
| Physical state | Liquid ^a |
| Melting point | 11.8 °C ^a |
| Boiling point | 101.1 °C ^a |
| Density | 1.0329 ^a |
| Odor | Faint pleasant odor ^a |
| Odor threshold: | |
| Water | No data |
| Air | 24 ppm v/v ^b |
| Taste | No data |
| Solubility: | |
| Water | Miscible ^c |
| Other solvents | Soluble in organic solvents ^a |
| Partition coefficients: | |
| Log K _{ow} | -0.27 ^d |
| Log K _{oc} | 1.23 ^b |
| Vapor pressure at 25 °C | 38.1 mm Hg ^e |
| OH radical rate constant | 1.09x10 ⁻¹¹ cm ³ /molecule-sec ^f |
| Henry's law constant at 25 °C | 4.80x10 ⁻⁶ atm-cm ³ /mole ^g |
| Autoignition temperature | 356 °F (180 °C) ^h |
| Flashpoint | 5–18 °C ^a |
| Flammability limits at 25 °C | Lower: 2.0%; Upper: 22% ^b |
| Incompatibilities | Strong oxidizers, decaborane, triethynyl aluminum ^h |
| Conversion factors (25 °C and 1 atm) | 1 ppm = 3.6 mg/m ³ ; 1 mg/m ³ = 0.278 ppm ^b |
| Explosive limits | Vapor forms explosive mixtures with air over wide range ⁱ |

^aO'Neil et al. 2001^bEC 2002^cRiddick et al. 1986^dHansch et al. 1995^eDaubert and Danner 1985^fAtkinson 1989^gPark et al. 1987^hNIOSH 2001ⁱNational Fire Protection Association 1997